Machine Learning

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Contents

1 Introduction

1.1 What is Machine Learning

1. Machine Learning
   - Grew out of work in Artificial Intelligence (AI)
   - New capabilities for computers
2. Examples:
   - database mining
   - applications can't programby hand (handwriting recognition, Natural Language Processing (NLP), Computer Vision)
   - Neuromorphic applications
3. Definition
   - Arthur Samuel(1959)

     > Machine Learning: Field of study that gives computers the ability to learn without being explicitly programmed.

   - Tom Mitchell(1998)

     > Well-posed Learning Problem: A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E.

4. Machine Learning in this course:
   (a) Suupervised Learning
   (b) Unsupervised Learning
   (c) Others: reinforcement learning, recommender systems
   (d) Practical application techniques

1.2 Supervised Learning

In supervised learning, the *the right answer* is given. For example:

1. Regression: predict real-valued output.
2. Classification: predict discrete-valued output.

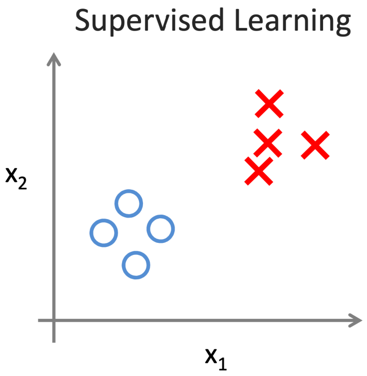


Figure 1: Supervised Learning

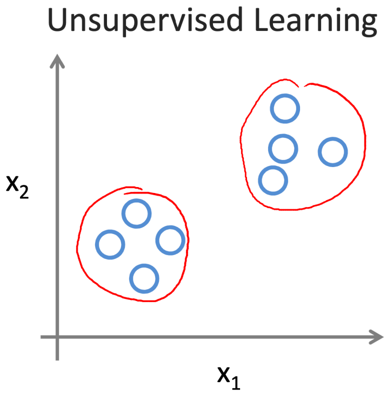


Figure 2: Unsupervised learning

1.3 Unsupervised Learning

The right answer is not given, e.g. cocktail problem (distinguishing two voices from an audio file.)

2 Linear Regression with One Variable

2.1 Model Representation

2.1.1 Notations

For a training set:

- **m** = Number of training examples.
- **x** = "input" variable / features.

- **y** = "output" variables / "target" variable.
- **(x,y)** - one training example.
- **($\mathbf{x^i}$,$\mathbf{y^i}$)** denotes the $\mathrm{i^{th}}$ training example

2.1.2 Hypothesis Function

A hypothesis function (h) maps input (x) to estimated output (y). How do we represent h?

$$\boxed{\textbf{Hypothesis Function} \quad h_\theta(x) = \theta_0 + \theta_1 x} \tag{1}$$

We can apply *Univariate linear regression* with respect to x.

2.2 Cost Function

Recall 1. The θ_is are parameters we have to choose. The intuition is is that we want to choose θ_i s such that h_θ is closest to y for our training examples (x,y).

$$\boxed{\textbf{Cost Function} \quad J(\theta_0, \theta_1) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2} \tag{2}$$

Summary

1. **Hypothesis** $h_\theta(x) = \theta_0 + \theta_1 x$
2. **Parameters** θ_0, θ_1
3. **Cost Function** $J(\theta_0, \theta_1) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$
4. **Goal** $\min_{\theta_0,\theta_1} J(\theta_0, \theta_1)$

2.3 Gradient Descent

2.3.1 Intuition

1. We have some function $J(\theta_0, \theta_1)$, we want to $\min_{\theta_0,\theta_1} J(\theta_0, \theta_1)$
2. Outline: start with some θ_0, θ_1, keep changing θ_0, θ_1 to reduce $J(\theta_0, \theta_1)$ until we end up at a minimum.

2.3.2 Gradient Descent Algorithm

Algorithm

repeat until convergence{

$$\theta_j := \theta_j - \alpha\frac{\partial}{\partial\theta_j}J(\theta_0, \theta_1) \quad \text{(for j=0 and j=1).}$$

}

Notes

1. the := denotes non-blocking assignment, i.e. simultaneously updates $\theta_0 and \theta_1$
2. We use the derivative to find a local minimum.
3. α denotes the learning rate. Gradient descent can converge to a local minimum even when the learning rate α is fixed. As we approach a local minimum, gradient descent will automatically take smaller steps. Therefore it is not needed to decrease α over time.

2.3.3 Gradient Descent with Linear Regression

Recall, we have:

1. Gradient Descent Algorithm:

   repeat until convergence{

   $$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \qquad \text{(for j=0 and j=1).}$$

   }

2. Linear Regression Model:

   $$h_\theta(x) = \theta_0 + \theta_1 x$$

   $$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

   We can substitute the above equations, which gives us:

   $$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})$$

   $$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x^{(i)}$$

3 Review of Linear Algebra

This is section is a basic review of linear algebra. I have skipped this section for now and will come back to it if time permits.

4 Linear Regression with Multiple Variables

4.1 Multiple features

Recall in the single variable case, we have a single input (x), two parameters(θ_0, θ_1). The hypothesis can be expressed as:

$$h_\theta(x) = \theta_0 + \theta_1 x.$$

Now, consider a generalized case where there are multiple features: X_1, X_2, X_3. The information can be organized in a table with example numerical values:

Sample Number (i)	X_1	X_2	y
1	6	87837	787
2	7	78	5415
3	545	778	7507
4	545	18744	7560
5	88	788	6344

Table 1: Sample Table

From Table 1, one can see that each row is a sample a feature on each column.

4.1.1 Notation

1. **n**: number of features.

2. $\mathbf{x^{(i)}}$: (row vector) input features of the i^{th} training example. i= 1, 2,. . . , m.

3. $\mathbf{x^{(i)}}_\mathbf{j}$: value of feature j in the i^{th} training example. j= 1, 2, . . . , n.

4.1.2 Hypothesis

Previously,

$$h_\theta(x) = \theta_0 + \theta_1 \cdot x$$

Now, we can extend the hypothesis to :

$$h_\theta(x) = \theta_0 \cdot 1 + \theta_1 \cdot x_1 + \theta_2 \cdot x_2$$

For convenience of notation, let's define x_0=1, i.e. ${x^i}_0$=1 ∀ i.

Therefore, we have: $\mathbf{x}= \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$ and $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}$. Then, the hypothesis function can be written as:

$$\begin{aligned} h_\theta(x) &= \begin{bmatrix} \theta_0 & \theta_1 & \theta_2 & \dots & \theta_n \end{bmatrix} \cdot \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \\ &= \theta^T \cdot \mathbf{x} \end{aligned} \tag{3}$$

This is *Multivariate linear regression.*

4.2 Gradient Descent for Multiple Variables

4.2.1 Algorithm

Summary for Multivariables

1. **Hypothesis** $h_\theta(x) = \theta^T \cdot \mathbf{x}$
2. **Parameters** θ
3. **Cost Function** $J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$
4. **Goal** $\min_\theta J(\theta)$

Gradient Descent for Multiple Variables

repeat until convergence {

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta) \qquad \text{(for j=0, 1,... n)}$$

}

$$\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^{m} (h_\theta(\mathbf{x}^{(\mathbf{i})}) - y^{(i)}) \cdot x_j^{(i)}$$

Note: $x_0^{(i)} = 1$, by definition.

4.2.2 Vectorized Implementation

One can work out the linear algebra and arrive at the following simplification using vectorized operations. The cost function J can be expressed as:

$$J(\theta) = \frac{1}{2m}(\mathbf{X}\theta - \mathbf{y})^T(\mathbf{X}\theta - \mathbf{y}) \tag{4}$$

The MATLAB implementation is as follows:

```
m = length(y); % calculate how many samples
J = 1/(2*m)*((X*theta-y).')*(X*theta-y);
```

Gradient descent can be vectorized in the form:

$$\theta = \theta - \frac{\alpha}{m} \cdot \mathbf{X}^T \cdot (\mathbf{X}\theta - \mathbf{y}) \tag{5}$$

The MATLAB implementation is as follows:

```
m = length(y); % number of training examples
for iter = 1:num_iters
    theta = theta - alpha/m* X.'*(X*theta -y);
```

4.3 Gradient Descent in Practise I: Feature Scaling

- Idea: ensure each featurre are on a similar scale
- Get every feature into approx. $-1 \leq x_i \leq 1(\sim \text{order})$
- **Mean Normalization**: Replace x_i with $\frac{x_i - \mu_i}{s_i}$, where μ_i and s_i are the sample mean and standard deviation, respectively.

4.4 Gradient Descent in Practise II: Learning Rate

- Ensure gradient descent is working: plot J_θ over each number of iteration (not over θ !)
- Example automatic convergence test: for sufficiently small α J_θ should decrease by less than 10^{-3} i one iteration.
- If α is too small, gradient descent can be slow to converge.
- If α is too large, gradient descent may not converge.
- To choose α, try 0.001, 0.003, 0.01, 0.03, 0.1, 0.3, 1... (by 3x)

4.5 Features and Polynomial Regression

We can fit into different polynomials by choice, using multivariate regression. Recall

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$

Let x_1 be x^1, x_2 be x^2, x_3 be x^3. Note we should still apply feature scaling to x_1, x_2, and x_3 individually!

4.6 Normal Equation

The normal equation provides a method to solve for θ analytically. For our data with m samples, n features, recall each sample can be written as:

$$\mathbf{x^{(i)}} = \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ x_2^{(i)} \\ \vdots \\ x_j^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix}$$

We can construct a design matrix:

$$\mathbf{X} = \begin{bmatrix} — & (x^{(1)})^T & — \\ — & (x^{(2)})^T & — \\ — & (x^{(3)})^T & — \\ & \vdots & \\ — & (x^{(m)})^T & — \end{bmatrix} \tag{6}$$

Then θ can be found by the normal equation:

$$\theta = (\mathbf{X^T X})^{-1}\mathbf{Ty} \tag{7}$$

Normal equation is useful as no α is required to and we do not need to iterate. However, we do have to compute $(X^T X)^{-1}$, which can be computationally expensive when n is large. The complexity is O(n^3) for inverse operations. Gradient Descent is useful when n is large (many features).

4.7 Normal Equation and Non-invertibility

What if $(X^T X)^{-1}$ is non-invertible?

- Redundant features (linearly dependent), i.e. having same information in two different units.
- Too many features (i.e. m $\leq$ n). Delete some features or use regularization

5 Octave/MATLAB Tutorial

6 Logistic Regression

6.1 Classification

- Binary Classification: y $\in \{0, 1\}$, where 0 denotes the negative class; 1 denotes the positive class.

- Multi-class Classification:y $\in \{0, 1, \cdots, n\}$

We will be using binary classification:

- Linear regression is not suitable for classification: since $h_\theta(x)$ can output out of range, i.e. < 0 or > 1.
- We will use **logistic regression**, which ensures that the output $h_\theta(x)$ is between 0 and 1.

6.2 Hypothesis Representation

6.2.1 Logistic function

The idea is to have $0 \leq h_\theta(x) \leq 1$. Instead of the linear regression hypothesis: $h_\theta(x) = \theta^T x$, we will let:

$$h_\theta(x) = g(\theta^t x),$$

where

$$g(z) = \frac{1}{1 + e^{-z}}$$

g(z) is known as the **logistic function**, also known as the Sigmoid function. Figure 3 shows a plot of the logistic function, which ranges from 0 to 1.

which yields

$$h_\theta(x) = \frac{1}{1 + e^{-z}} \tag{8}$$

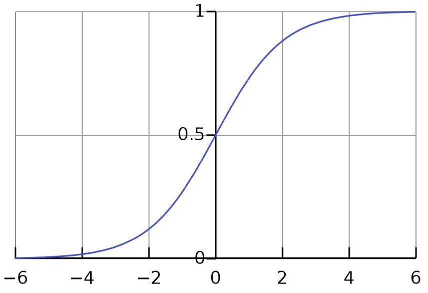


Figure 3: Sigmoid Function

6.2.2 Interpretation of Hypothesis Output

$h_\theta(x) =$ estimated probability that y$=$ 1 on input x. For example, $h_\theta(x) = 0.7$ gives us a probability of 70% that are output is 1. From a probability theory point of view, one can express $h_\theta(x)$ as $P(y = 1 \mid x; \theta)$.

Note that since this is a probability and the total probability sums up to 1, and the real y can only be either 0 or 1:

$$P(y = 0 \mid x; \theta) + P(y = 1 \mid x; \theta) = 1$$

6.3 Decision Boundary

Recall so far we have $h_\theta(x) = g(\theta^T x)$ and $g(z) = \frac{1}{1+exp(-z)}$. Suppose we set $h_\theta(x) = 0.5$ to be our determining factor for whether y= 0 or y =1. Note that from 3, one can observe that $h_\theta(x) = 0.5$ corresponds to $\theta^T x = 0$, which is the **decision boundary**. The decision boundary is the equation which separates the different classes on a plot. There are linear and non-linear decision boundaries.

6.4 Cost function

Previously, we had $J(\theta) = \frac{1}{m}\sum_{i=1}^{m} Cost(h_\theta(x^{(i)}), y^{(i)})$, where $Cost(h_\theta(x), y) = \frac{1}{2}(h_\theta(x) - y)^2$. Now, the definition of the hypothesis h_θ has changed to $\frac{1}{1+exp(-\theta^T x}$, as a result the cost function is now non-convex.

Logistic Regression Cost Function
Therefore, a new cost function definition is needed. We propose:

$$Cost(h_\theta(x), y) = \begin{cases} -log(h_\theta(x)) & \text{if } y = 1 \\ -log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$

Note that Cost=0, if y=1, $h_\theta(x) = 1$; but as $h_\theta(x) \to 0$, then $Cost \to \infty$. This proposition captures the intuition that if $h_\theta(x) = 0$, predict $P(y = 1 \mid x; \theta)$, but y ends up being 1, we will penalize the learning algorithm by very large cost.

6.5 Simplified Cost Function and Gradient Descent

Since y can only be either 0 or 1, we can simplify the cost function.

$$\begin{aligned} J(\theta) &= \frac{1}{m}\sum_{i=1}^{m} Cost\,(\,h_\theta(x^{(i)})\,,\,y^{(i)}) \\ &= \frac{-1}{m}\,[\,\sum_{i=1}^{m} y^{(i)}\,log\,h_\theta(x^{(i)}) \;+\; (1 - y^{(i)})\,log\,(\,1 - h_\theta(x^{(i)})\,)\,] \end{aligned} \tag{9}$$

Equation 9 is based on Maximum Likelihood Estimation.

A vectorized implementation is, for a design matrix **X**:

$$\boxed{h = g(\mathbf{X}\theta)} \tag{10}$$

$$\boxed{J(\theta) = \frac{1}{m}(-y^T log(h) - (1 - y)^T log(1 - h))} \tag{11}$$

For gradient descent,we would want to $\min_\theta J(\theta)$:

Repeat {

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

}

We can compute the partial derivative of $J(\theta)$, which is identical to that of linear regression:

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \cdot x^{(i)}$$

However, in this case the hypothesis function $h_\theta(x) = \frac{1}{1+exp(-\theta^T x}$ has changed!

A vectorized implementation for this is:

$$\boxed{\theta := \theta - \frac{\alpha}{m} \mathbf{X}^T (g(\mathbf{X}\theta) - \mathbf{y}))} \tag{12}$$

6.6 Advanced Optimization

6.6.1 Taking a Step Back

If we take a step back, and consider essentially what tasks we are performing. We need to compute two things:

1. $J(\theta)$
2. $\frac{\partial}{\partial \theta_j} J(\theta)$

6.6.2 Optimization Algorithm

There exists other more sophisticated and faster ways to optimize θ instead of gradient descent; they often do not involve selecting learning rate α and are more efficient. However, these algorithms are harder to code by hand. It is suggested that we use libraries for such algorithms.

We can write a single function that returns both $J(\theta)$ (jVal) and $\frac{\partial}{\partial \theta_j} J(\theta)$ (gradient):

```
function [jVal, gradient] = costFunction(theta)
    jVal = [...code to compute J(theta)...];
    gradient = [...code to compute derivative of J(theta)...];
end
```

Then we can use octave's "fminunc()" optimization algorithm along with the "optimset()" function that creates an object containing the options we want to send to "fminunc()".

```
    options = optimset('GradObj', 'on', 'MaxIter', 100);
    initialTheta = zeros(2,1);
    [optTheta, functionVal, exitFlag] = fminunc(@costFunction,
        initialTheta, options);
```

We then give to the function "fminunc()" our cost function, our initial vector of theta values, and the "options" object that we created beforehand.

6.7 Multiclass Classification: One-vs-All

Now, let's extend the binary classification of data to multi-classes, i.e expanding our definition of y s.t. y={0, 1, . . . , n}. We will divide out problem into n+1 (0. . . n) binary classification problems. In each problem, we predict the probability that y is a memember of one of our class. We train a logistic regression classifier $h_\theta^{(i)}(x)$ ∀ i to predict y = i:

$$h_\theta^{(i)}(x) = P(y = i \mid x; \theta) \tag{13}$$

Figure 4 shows an example of the procedure of classifying three classes. We choose one class and then lump all the others into a single second class (hence the name One-vs-All). We apply the binary logisic regression repeatedly and use the hypothesis that returns the highest value.

$$prediction \;=\; \max_i\,(\,h_\theta^{(i)}(x)\,) \tag{14}$$

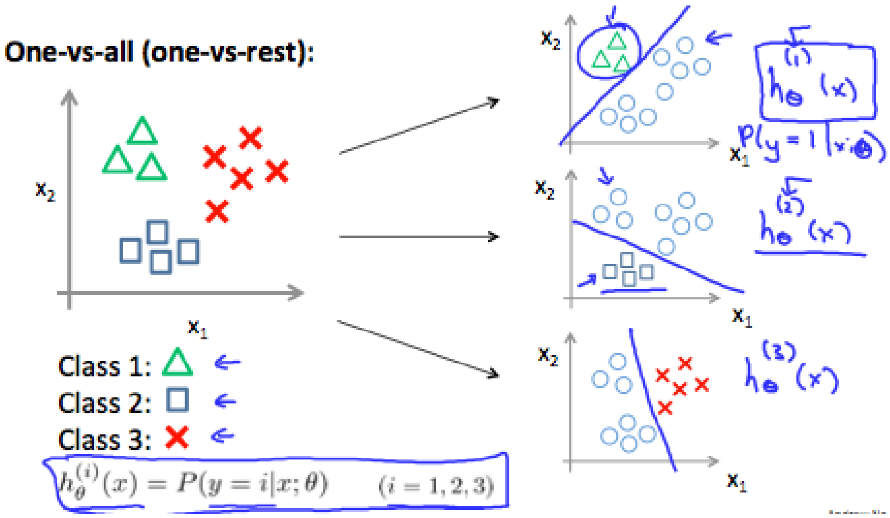


Figure 4: Example of Multiclass Logistic Regression

7 Regularization

7.1 The problem of overfitting

There are two types of errors in fitting functions to data, in which data shows the structure is not captured by the model. The terminology applies to both linear and logistic regression. Figure 5 shows an example of each fitting case.

1. Underfitting (high bias): when the form of our hypothesis function ($h_\theta(x)$) maps poorly to the trend of data. It is usually caused by a function that is either too simple or uses too little features.
2. Overfitting (high variance): when hypothesis function learns the training set very well hence fits the available data but does not generalize well to predict new data, i.e fitting too many details. It is usually caused by a complicated function that creates a lot of unneccessary curves and angles unrelated to the data.

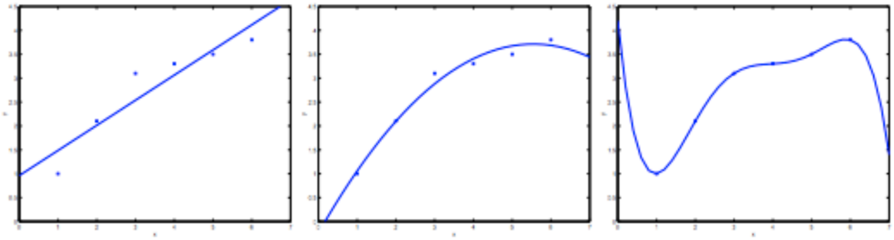


Figure 5: Three scenarios of fitting: underfit(left), good fit (middle), and overfit(right).

There are two main options to address the issue of overfitting:

1. Reduce the number of features
   - manually select which features to keep.
   - Use a model selection algorithm (later in the course).
2. **Regularization**
   - Keep all the features, but reduce the magnitude of parameters θ_j
   - Regularization worls well when we have a lot of slightly useful features. (Each contributes a bit to predict y)

7.2 Cost Function

7.2.1 Intuition

Suppose we have overfitting, we can reduce the weight that some of the terms in our function carry by penalizing the feature parameter with increased cost. Consider the following hypothesis function :

$$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta x^3 + \theta x^4.$$

We would want to make the function more quadratic, which means we would like to reduce the influence of θ_3 and θ_4. Since our goal was to minimize the cost function $J(\theta)$, we could modify the original cost function

$$\min_\theta \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + 1000 \cdot \theta_3^2 + 1000 \cdot \theta_4^2.$$

This will force θ_3 and θ_4 to be close to zero, and make the original hypothesis function more quadratic.

7.2.2 Regularization

Now, we can take a step further and regularize all theta parameters:

$$\min_\theta \ [\frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2] + \lambda\sum_{j=1}^{n}\theta_j^2 \tag{15}$$

Here we are performing two separate operations which can be oberved as the two terms in Equation 15. The first term corresponds to “training the data”, and the second term relates to “keeping the parameters small”. The coefficient λ is the **regularization parameter** and determines the balance between the aforementioned two objectives. Note that if λ is too big ($\approx 10^{10}$), then all $\theta_j \approx 0$, except for θ_0 (the constant term). This makes $h_\theta \approx 0$ and defies the purpose of training and leads to underfitting (a flat horizontal line).

7.3 Regularized Linear Regression

7.3.1 Gradient Descent

We will modify the gradient descent function to separate out θ_0 from the rest of the parameters because we do not want to penalize θ_0.

repeat until convergence{

$$\theta_0 := \theta_0 - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha[(\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}) + \frac{\lambda}{m}\theta_j]$$

} , where $j \in \{1, 2, \ldots, n\}$

The above equation can be re-arranged to get the final form:

$$\boxed{\theta_j := \theta_j(1 - \alpha\frac{\lambda}{m}) - \frac{\alpha}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}} \tag{16}$$

The term $(1 - \alpha\frac{\lambda}{m})$ will always be less than 1. Intuitively, this reduces the parameter, then the rest of equation 16 carries the normal gradient descent.

7.3.2 Normal Equation

Recall from our previous normal equation (Equation 7), we have the design matrix $\mathbf{X}$ such that

$$\mathbf{X} = \begin{bmatrix} — & (x^{(1)})^T & — \\ — & (x^{(2)})^T & — \\ — & (x^{(3)})^T & — \\ & \vdots & \\ — & (x_m^T & — \end{bmatrix}$$

Now, to add in regularization to Equation 7, we get:

$$\boxed{\theta = ((\mathbf{X}^{\mathbf{T}}\mathbf{X}) + \lambda \cdot \mathbf{L})^{-1}\mathbf{x}^T y} \tag{17}$$

where $L \in \mathbb{R}^{(n+1)\times(n+1)}$

$$L = \begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix} \tag{18}$$

Supopose non-invertibility arises: $m \leq n$, i.e #examples is less than or equal to number of features, then using a $\lambda > 0$ in Equation 17 will resolve the non-invertibility.

7.4 Regularized Logistic Regression

7.4.1 Regularized Logistic Cost Function

We can modify our old logistic cost function (Equation 9) to apply regularization.

$$\boxed{J(\theta) = \frac{-1}{m}\sum_{i=1}^{m}[y^{(i)}\, log\, h_\theta(x^{(i)}) \ + \ (1 - y^{(i)})\, log\,(\,1 - h_\theta(x^{(i)})\,)] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2} \tag{19}$$

Note that the second sum in Equation 19 explicitly exludes the bias term θ_0.

7.4.2 Regularized Logistic Gradient Descent

The gradient descent is similar to that of linear regression; however note that the hypothesis function has been updated to Equation 8.

repeat until convergence{

$$\theta_0 := \theta_0 - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_0^{(i)}$$

$$\theta_j := \theta_j - \alpha[(\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}) + \frac{\lambda}{m}\theta_j]$$

}

8 Neural Networks: Representation

8.1 Non-linear Hypothesis

- Example: non-linear classification- logistic regression has lots of terms and not scalable($O(n^2), O(n^3)$).
- Application: computer vision
- Neural network is useful for **non-linear, large scale classification**.

8.2 Neurons and the brain

- Origin: Neuromorphic computing mimics how brain functions.
- Recent resurgence due to hardware advancement.
- The "one-learning hypothesis": there exists a single algorithm that the brain uses for generalized learning.
  - Neural re-wiring: wiring the auditory cortex to eyes, then the cortex learns how to *see*.

8.3 Model representation

Figure 6 shows a model of a biological neuron. The **dendrites** are the wires which receive input signal. The **axons** output the signal.

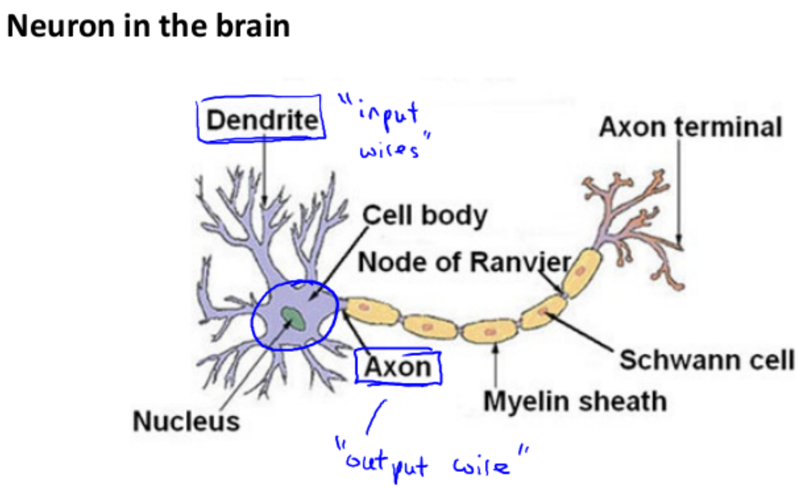


Figure 6: A biological neuron

8.3.1 Neural model: logistic unit

In our model:

- Dendrites: input features $\mathrm{x_1}$, $\mathrm{x_2}$, ..., $\mathrm{x_n}$.
- Output: result of hypothesis function.
- $\mathrm{x_0}$: bias unit (:= 1).
- Logistic function: $\frac{1}{1+exp(-\theta^T X)}$, referred to as the sigmoid(logistic) **activation** function.
- θ are referred to as **weights**.

Visually, a simplistic representation can be view as

$$[x_0\ x_1\ x_2] \ \rightarrow \ [\,] \ \rightarrow \ h_\theta(x) \tag{20}$$

The input nodes (layer 1, input layer) go into the another node (layer 2), which then outputs to hypothesis function (output layer).

In this example, we label the intermediate layers of nodes (between the input and output layers) $a_0^2, \ldots, a_n^2$: **activation units**. Definitions:

$a_i^{(j)}$ = "activation of unit i in layer j

$\Theta^{(j)}$= matrix of weights controlling function mapping from layer j to layer j+1.

If we had one hidden layer, it would look like:

$$\boxed{[x_0\, x_1\, x_2\, x_3] \;\rightarrow\; [a_1^{(2)}, a_2^{(2)}, a_3^{(2)}] \;\rightarrow h_\theta(x)}$$

The value for each of the activation node is obtained as follows;

$$a_1^{(2)} = g(\Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3)$$

$$a_2^{(2)} = g(\Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3)$$

$$a_3^{(2)} = g(\Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3)$$

$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(1)}a_0 + \Theta_{11}^{(1)}a_1 + \Theta_{12}^{(1)}a_2 + \Theta_{13}^{(1)}a_3)$$

Essentially, each layer j has its own **matrix of weights**, $\Theta^{(j)}$.

If network has s_j units in layer j and s_{j+1} units in layer j+1, then $\Theta^{(j)}$ will be of dimension $s_{j+1} \times (s_j + 1)$.

The $+1$ comes from the addition in $\Theta^{(j)}$ of the bias nodes, x_0 and $\Theta_0^{(j)}$.

In the above example, layer 2 has 3 units ($a_1^{(2)}, a_2^{(2)}, a_3^{(2)}$) and layer 1 has 3 units (not including the bias unit). Therefore the weight matrix $\Theta^{(1)}$ which maps layer 1 to layer 2 is of dimension $3 \times (3 + 1)$.

Another example: if layer 1 has 2 input nodes and layer 2 has 4 activation nodes- dim ($\Theta^{(1)}$) is going to be 4x3 where $s_j = 2$ and $s_{j+1} = 4$, so $s_{j+1} \times (s_j + 1) = 4 \times 3$.

8.3.2 Forward Propagation: Vectorized Implementation

Define a new variable: $z_k^{(j)}$ as the parameter for for the logistic function $g(z)$ such that:

$$a_1^{(2)} = g(z_1^{(2)})$$
$$a_2^{(2)} = g(z_2^{(2)})$$
$$a_3^{(2)} = g(z_3^{(2)})$$

Therefore, for layer j=2 and unit k:

$$z_k^{(2)} = \Theta_{k,0}^{(1)}x_0 + \Theta_{k,1}^{(1)}x_1 + \cdots + \Theta_{k,n}^{(1)}x_n$$

$$x = \begin{bmatrix} x_0 \\ x_1 \\ \cdots \\ x_n \end{bmatrix} \; z^{(j)} = \begin{bmatrix} z_1^{(j)} \\ z_2^{(j)} \\ \cdots \\ z_n^{(j)} \end{bmatrix}$$

We can further generalize by setting $\mathbf{x} = a^{(1)}$ and re-write the equation:

$$z^{(j)} = \Theta^{(j-1)}a^{(j-1)} \tag{21}$$

Dimension check:

- $\Theta^{(j-1)}$ is of dimension $s_j \times (n+1)$.
- a$^{\text{(j)}}$ is a column vector with dimension $1 \times (j+1)$.

Thus the logistic function is applied element-wise to **z**:

$$a^{(j)} = g(z^{(j)}) \tag{22}$$

We then add the bias unit $a_0^{(j)} = 1$ to the activation matrix. If we propagate forward by one layer in Equation 21:

$$z^{(j+1)} = \Theta^{(j)} a^{(j)} \tag{23}$$

The last theta matrix $\Theta^{(j)}$ will have only one row which is multiplied by one column $a^{(j)}$ such that the result is a single scalar.Hence the final hypothesis output is:

$$h_\theta(x) = a^{(j+1)} = g(z^{(j+1)}) \tag{24}$$

8.4 Application - Logic Gate Synthesis

We can apply neural networks to predict various logic gates: AND, OR, XOR, NOR. The basic graph can be represented as :

$$\begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} \rightarrow \ [\ g(z^{(2)})\ ] \rightarrow \ h_\Theta(x)$$

8.4.1 AND Gate

Let the first theta matrix be:

$$\Theta^{(1)} = [\ -30\ \ 20\ \ 20\ \ ]$$

Table 2 outlines the logistic hypothesis output which represents an AND gate: output = 1 $\iff$ ($x_1 = 1$ and $x_2 = 1$). The intuition here in choosing the Θ parameters is that we want the sigmoid function evaluate to be positive only when both x$_1$ and x$_2$ are logic 1. Therefore, we assign the bias unit to a large negative value, such that the result of Θx is positive only when both the two other weights are added.

8.4.2 OR Gate

Similarly, Table 3 outlines the truth table for the OR function. We pick a parameter matrix:

$$\Theta^{(1)} = [\ -10\ \ 20\ \ 20\ \ ]$$

x_1	x_2	z	$h_\Theta(x) = g(z)$
0	0	-30	0
0	1	-10	0
1	0	-10	0
1	1	10	1

Table 2: Truth table of AND gate

x_1	x_2	z	$h_\Theta(x) = g(z)$
0	0	-10	0
0	1	10	1
1	0	10	1
1	1	30	1

Table 3: Truth table of OR gate

8.4.3 NOR Gate

Similarly, Table 4 outlines the truth table for the NOR function. We pick a parameter matrix:

$$\Theta^{(1)} = [\ 10 \quad -20 \quad -20\ ]$$

8.4.4 NOT Gate

For an inversion, we just need a single parameter x. Table 5 outlines the truth table for the NOT function. We pick a parameter matrix:

$$\Theta^{(1)} = [\ 10 \quad -20\ ]$$

8.4.5 XNOR Gate

Now, we would like to synthesize the XNOR function (shown in Table 6. This requires a three level neural network. We can decompose the function XNOR:

$$\overline{x_1 \oplus x_2} = x_1 x_2 + \overline{x_1} \cdot \overline{x_2}$$

x_1	x_2	z	$h_\Theta(x) = g(z)$
0	0	10	1
0	1	-10	0
1	0	-10	0
1	1	-30	0

Table 4: Truth table of NOR gate

x	z	$h_\Theta(x) = g(z)$
0	10	1
1	-10	0

Table 5: Truth table of NOT gate

x_1	x_2	$a_1^{(2)}$	$a_2^{(2)}$	$h_\Theta(x)$
0	0	0	1	1
0	1	0	0	0
1	0	0	0	0
1	1	1	0	1

Table 6: Truth table of XNOR

Therefore, in the second layer we will computer the AND and NOR functions then apply OR to the two intermediate output in the third layer.

$$\Theta^{(1)} = [\ -30\ \ 30\ \ 20\ \ ]$$

$$\Theta^{(2)} = [\ -10\ \ 20\ \ 20\ \ ]$$

So:

$$a^{(2)} = g(\Theta^{(1)} \cdot x)$$
$$a^{(3)} = g(\Theta^{(2)} \cdot a^{(2)})$$
$$h_\Theta(x) = a^{(3)}$$

8.5 Multi-class Classification

For multi-class classification, our prediction will be a column vector with each element be of "whether the current item belongs to the class of that position". For example, for a 4-class classification, an example output would be:

$$h_\Theta(x) = [0010]$$

9 Neural Networks: Learning

9.1 Cost Function

Define variables:

- L :total number of layers in the network.
- s_l: number of units (not counting bias unit) in layer l.

- K: number of output classes.

Recall for classifications, we have binary and multi-class:

1. Binary classification:
   - y = 0 or 1.
   - 1 output unit, i.e. $h_\Theta(x) \in \mathbb{R}$.
   - $S_L = 1$; K = 1.
2. Multi-class classification:
   - $y \in \mathbb{R}^K$
   - $S_L = K$. $K \geq 3$.

Recall the cost function for regularized logistic regression in Equation 19, shown below:

$$J(\theta) = \frac{-1}{m} \sum_{i=1}^{m} [y^{(i)}\, log\, h_\theta(x^{(i)}) \;+\; (1 - y^{(i)})\, log\,(\, 1 - h_\theta(x^{(i)})\,)] + \frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2$$

For neural networks, we will extend Equation 19 into a generalized form:

$$\begin{aligned} J(\Theta) = & \frac{-1}{m} \sum_{i=1}^{m} \sum_{k=1}^{K} [y_k^{(i)}\, log\, h_\theta(x^{(i)})_k \;+\; (1 - y_k^{(i)})\, log\,(\, 1 - h_\theta(x^{(i)})_k\,)] \\ & + \frac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_l} \sum_{j=1}^{s_{l+1}} (\Theta_{j,i}^{(l)})^2 \end{aligned} \tag{25}$$

In the first part of Equation 25, we added a summation to account for multiple output nodes. Note:

- Double sum adds up logistic regression costs calculated for each cell in the output layer.
- Triple sum adds up the squares if all individuals Θs in the entire network.
- The i in the triple sum does not refer to the training example i !

9.2 Backpropagation Algorithm

- Backpropagation: neural-network terminology for minimizing cost function.
- Gradient Computation: need to computer $J(\Theta)$ and $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$

Given a training set { $(x^{(1)}, y^{(1)}) \ldots (x^{(m)}, y^{(m)})$}. Set $\Delta_{i,j}^{(l)} = 0$ ∀ l,i,j.

For all training examples t=1:m:

1. Set $a^{(1)} := x^{(t)}$
2. Perform forward propagation to computer all the nodes ($a^{(l)}$).
3. Using $y^{(t)}$, compute $\delta^{(L)} = a^{(L)} - y^{(t)}$. (Vectorized deviation of output units to correct values).
4. Backpropagate the error:

   $$\delta^{(l)} = ((\Theta^{(l)})^T \delta^{(l+1)}).*a^{(l)}.*(1 - a^{(l)})$$

   This equation makes use of the fact that the derivative of the sigmoid function:

   $$g'(z^{(l)}) = a^{(l)}.*(1 - a^{(l)})$$

5. Obtain the estimation of gradient ($\nabla J(\Theta)$). Intuitively, $\delta^{(l)}$ is the error for the activation unit in layer l: a^{l}. more formally, the delta values are the derivatives of the cost functions.
   It can be shown that

   $$\boxed{\frac{\partial}{\partial \Theta_{i,j}^{(l)}} J(\Theta) = a_j^{(l)} \cdot \delta_i^{(l+1)}}$$

   Hence, a vectorized implementation of the accumulated gradient is:

   $$\Delta^{(l)} := \Delta^{(l)} + \delta^{(l+1)}(a^{(l)})^T$$

We then normalize and add regularization to obtain the gradient:

- $D_{i,j}^{(l)} := \frac{1}{m}(\Delta_{i,j}^{(l)} + \lambda \Theta_{i,j}^{(l)})$, if j $\neq$ 0
- $D_{i,j}^{(l)} := \frac{1}{m}\Delta_{i,j}^{(l)}$, if j=0

And thus $\frac{\partial}{\partial \theta^{(l)}} = D^{(l)}$.

9.3 Gradient checking

- Purpose: Eliminates error from escaping. Assuring backpropagation is working as intended.
- Approx derivative as:

  $$\frac{\partial}{\partial \Theta_j} J(\Theta) \approx \frac{J(\Theta_1, \ldots, \Theta_j + \epsilon, \ldots, \Theta_n) - J(\Theta_1, \ldots, \Theta_j - \epsilon, \ldots, \Theta_n)}{2\epsilon}$$

- Compute the gradient approximation and compare with backpropagation(delta vector)
- Turn off gradient checking as this is computationally expensive.

Below is an implementation of gradient checking in MATLAB code:

```
epsilon = 1e-4;
for i = 1:n,
  thetaPlus = theta;
  thetaPlus(i) += epsilon;
  thetaMinus = theta;
  thetaMinus(i) -= epsilon;
  gradApprox(i) = (J(thetaPlus) - J(thetaMinus))/(2*epsilon)
end;
```

9.4 Random Initialization

- Initializing all theta weights to zero does not work. In backpropagation, all nodes will update to the same value repeatedly, creating **symmetry**.
- Symmetry breaking: initialize to values that range in [-ϵ, ϵ]

10 Advice for Applying Machine Learning

10.1 Deciding What to Try Next

Potential next steps:

1. Larger training data.
2. Smaller set of feature.
3. Additional features.
4. Polynomial features.
5. Increase λ.
6. Decrease λ.

Machine Learning Diagnostic: a test to run to gain insight on feasibility of techniques and how to optimize performance.

10.2 Evaluating Hypothesis: training/validation/test sets

10.2.1 Motivation with Test sets

We want to address the problem of overfitting: fits training examples very well (low error) but fails to generalize and hence not inaccurate on additional data. Thus, to evaluate the true accuracy of hypothesis, we randomly split the data into two sets: a **training set** (70%) and a **test set** (30%). The procedure :

1. Learn Θ and minimize $J_{train}(\Theta)$ using the training set

2. Compute test set error: $J_{test}(\Theta)$.

   (a) For linear regression:

   $$J_{test}(\Theta) = \frac{1}{2m_{test}} \sum_{i=1}^{m_{test}} (h_\theta(x_{test}^{(i)}) - y_{test}^{(i)})^2$$

   (b) For logistic regression:

   $$J(\theta) = \frac{-1}{m_{test}} \sum_{i=1}^{m_{test}} (y_{test}^{(i)} log(h_\Theta(x_{test}^{(i)}) + (1 - y_{test}^{(i)}) log(1 - h_\Theta(x_{test}^{(i)}))$$

   (c) For classification, we first calculate the misclassification error.

   $$err(h_\Theta(x), y) = \begin{cases} 1 & \text{if } (h_\Theta(x) \geq 0.5 \text{ \& } y = 0) \text{ or } (h_\Theta(x) \leq 0.5 \text{ \& } y = 1) \\ 0 & \text{if otherwise.} \end{cases} \tag{26}$$

   The average test error is thus:

   $$\text{Test error} = \frac{1}{m_{test}} \sum_{i=1}^{m_{test}} err(h_\Theta(x), y) \tag{27}$$

10.2.2 Polynomial features: Train/Validation/Test model

- Computed cost is less than the generalization error: We trained our data on the training set to obtain Θ with different degrees of polynomial (d). We then choose d based on minimizing the test set.
- Problem: $J_{test}(\Theta)$ is likely to be an optimistic generalization error, since the parameter d is fit to the test data set.
- Solution: break down dataset into three sections:
  1. Training set (60%).
  2. Cross-validation set (20%).
  3. Test set (20%).

Procedure:

1. Optimize the parameters in Θ using the training set for each polynomial degree.
2. Find the polynomial degree d with the least error using the cross validation set.
3. Estimate the generalization error using the test set with $J_{test}(\Theta^{(d)})$, (d = theta from polynomial with lower error);

This way, the degree of the polynomial d has not been trained using the test set.

10.3 Diagnosing Bias vs Variance

- Degree of polynomial (d) and underfitting (high bias) / overfitting (high variance).
- Training errors tend to decrease as d increases.
- Cross validation error tends to form a convex curve with a minimum point.

Therefore, the key to distinguish between bias and variance is summarized in Figure 7.

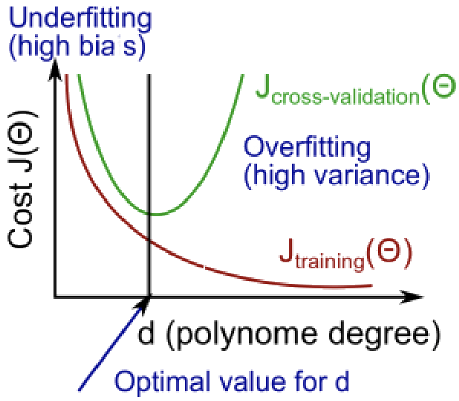


Figure 7: Error cost of cross-validation and training over degree of polynomial

1. **High bias (underfitting)**: both $J_{train}(\Theta)$ and $J_{CV}(\Theta)$ will be high. Thus: $J_{train}(\Theta) \approx J_{CV}(\Theta)$
2. **High variance (overfitting)**: *Low* $J_{train}(\Theta)$ and *high* $J_{CV}(\Theta)$. Thus: $J_{train}(\Theta) << J_{CV}(\Theta)$

10.4 Regularization and bias and variance

- Large λ (lower significance of Θ, heavy penalization so $h_\theta \approx 0$): high bias, underfit.
- Small λ (high significance of Θ): high variance, overfit.

Procedure to pick the right λ:

1. Create list of lambda.
2. Iterate through λs and learn/obtain Θ.
3. Compute cross-validation error ($J_{CV}(\Theta)$) using the learned Θ **without regularization** (i.e. $\lambda = 0$)
4. Select the best lambda and Theta pair and verify on test set. (Compute $J_{test}(\Theta)$.

10.5 Learning Curves

Plotting error over number of training examples.

10.5.1 High bias

1. Low training set size: low J_{train} and high J_{CV}.
2. Large training set size: high J_{train} and high J_{CV}.

Getting more training data will not help.

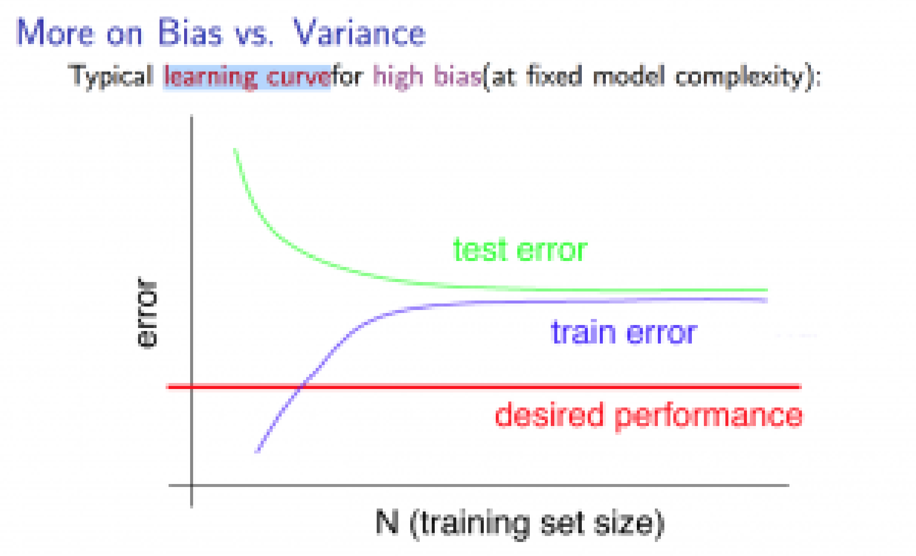


Figure 8: Learning curve for high bias

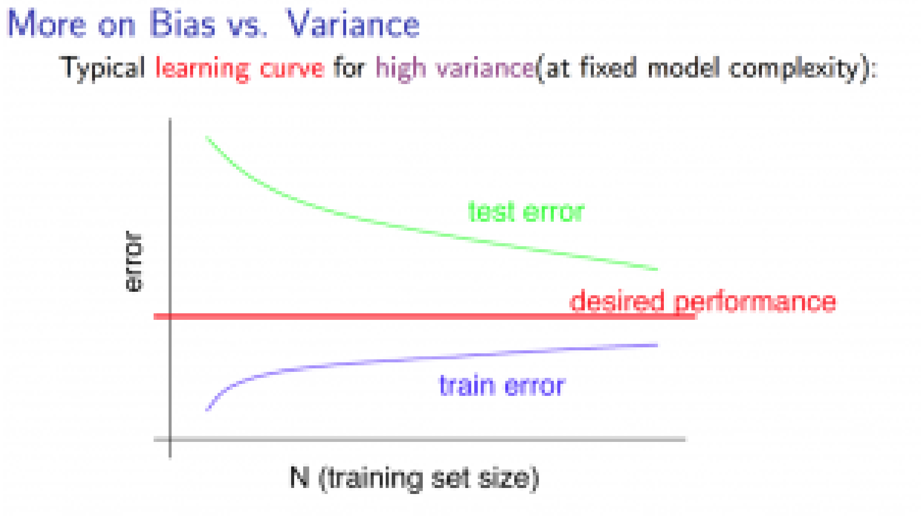
10.5.2 High variance

1. Low training set size: low J_{train} and high J_{CV}.
2. Large training set size: J_{train} increases and J_{CV} decreases.

Getting more training data will help.

10.6 Summary

1. Getting more training examples: Fixes high variance
2. Trying smaller sets of features: Fixes high variance
3. Adding features: Fixes high bias



More on Bias vs. Variance

Typical learning curve for high variance(at fixed model complexity):

Figure 9: Learning curve for high variance

4. Adding polynomial features: Fixes high bias
5. Decreasing λ: Fixes high bias
6. Increasing λ: Fixes high variance.

10.7 Neural Networks

1. Small neural network: fewer parameters $\implies$ prone to underfitting, but computationally cheaper.
2. Large neural network: more parameters $\implies$ prone to overfitting, computationally expensive. Use regularization to address overfitting.

11 Machine Learning System design

11.1 Prioritizing what to work on: Spam Classification Example

- Supervised learning.
- $\mathbf{x}$ = features of email (words indicative of spam).
- y = 1 (spam) or 0 (not spam).
- In practise, we take the most frequent n words (10000 to 50000) in training set to use as elements in x.

Potential next steps:

1. Collect lots of data.
2. Develop sophisticated features, e.g. for email routing information, message body, etc.
3. Sophisticated algorithms.

11.2 Error Analysis

11.2.1 Recommended Approach

- Start with simple algorithm that can be implemented quickly. Implement and test on *Cross-validation data.*
- Plot learning curves to decide if more data or more features will help.
- Error analysis: Manually examine errors from the examples in *cross-validation* set. Observe any systematic trend.

11.2.2 Error Analysis

Questions to ask:

1. What type of email it is.
2. What cues (features) do you think would have helped the algorithm to classify them correctly.

11.2.3 The importance of numerical evaluation

- Should discount/discounts/discounted/discounting be treated as the same word?
  - Use "stemming" software, e.g. *Porter Stemmer*
- Error analysis might not help. Instead, try and see it it works.
- Need metric (numerical evaluation) of algorithm to evaluate performance. E.g. cross validation error.

11.3 Error Metrics for Skewed Classes

11.3.1 Motivation

Consider case for cancer classification. If we get 1% error on the test set, i.e. 99% diagnoses are correct. However, only 0.5% of patients have cancer in the first place. Is the 1% error a good evaluation? Furthermore, consider the example prediction algorithm:

```
function y = predictCancer(x)
    y=0; %ignore x!
return
```

Regardless of the dataset, the hypothesis will always predict y=0.

11.3.2 Precision/Recall

	Actual	1	0
Prediction	1	True positive	False positive
	0	False negative	True negative

Table 7: Truth Table

We can thus define two measures of accuracy:

$$\textbf{precision} = \frac{\text{True pos}}{\text{No. of predicted pos}} = \frac{\text{True pos}}{\text{True pos} + \text{False pos}} \tag{28}$$

$$\textbf{recall} = \frac{\text{True pos}}{\text{No. of actual pos}} = \frac{\text{True pos}}{\text{True pos} + \text{False neg}} \tag{29}$$

Convention: Define y=1 in presence of *rare class* that we want to detect.

11.4 Trading off Precision and Recall

Recall that for logistic regression, we have the hypothesis $0 \leq h_\theta(x) \leq 1$. Note that earlier we set the threshold to be 0.5. Now we can set the threshold higher (e.g, 0.8 for a more confident prediction), or lower (e.g. 0.3 for a greater coverage).

Consider two use cases:

1. Suppose we want to predict y=1 (cancer) only if we are very confident: We will set the threshold to be high.
   High precision, low recall.

2. Suppose we want to avoid missing too many cases of cancer (avoid false negatives): We will set the threshold to be low.
   High recall, low precision.

11.4.1 F$_1$ score

Now that we have two metrics, precision and recall, we need a method to combine the two into a single metric evaluation for comparison purposes. An initial step may be to use the arithmetic mean. However, this can be inaccurate when either precision or recall is extremely high and the other extremely low. The mean will yield a somewhat high value. We need a better metric. Here we propose the F$_1$ score:

$$F_1 = 2\,\frac{PR}{P+R} \tag{30}$$

11.5 Large Data Rationale

At some point, we will need to acquire more data. A larger dataset is useful when $x \in \mathbb{R}^{n+1}$ has sufficient information to predict y accurately. A useful mental test is: given the input x, can a human expert confidently predict y?

When we use a learning algorithm with many parameters, e.g. logistic regression, linear regression with many features; neural network with many hidden units. This ensures a low bias algorithm. Therefore $J_{train}(\Theta)$ will be small.

Now, we can then use a large training set (which is unlikely to overfit) and ensure low variance. In such case, $J_{train}(\Theta) \approx J_{test}(\Theta)$, which makes the test error low.

12 Support Vector Machine

12.1 Optimization Objective

12.1.1 Alternative View of Logistic Regression

$$h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$$

If y = 1, we want $h_\theta(x) \approx 1$, $\theta^T x >> 0$.
If y = 0, we want $h_\theta(x) \approx 0$, $\theta^T x << 0$
Cost of example:

$$\boxed{y\ log\ h_\theta(x) \ + \ (1-y)\ log(1-h_\theta(x))) \ = \ -y\ log\ \frac{1}{1\ +\ e^{-\theta^T x}} \ - \ (1-y)\ log\ (1-\frac{1}{1+\ e^{\theta^T\ x}})}$$

Consider the two terms in the above equation, where now we replace the cost with a straightened two-section curve:

1. If y=1 , want $h_\theta(x) \approx 1$, $\theta^T x >> 0$. Here we label the curve as cost$_0$ (z), as shown in Figure 10.
2. If y = 0, we want $h_\theta(x) \approx 0$, $\theta^T x << 0$. Here we label the curve as cost$_1$(z), as shown in Figure 11..

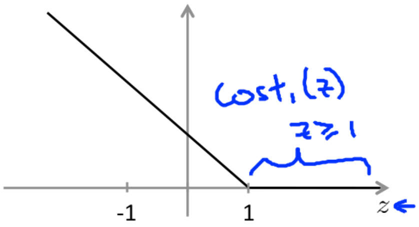


Figure 10: SVM cost_1

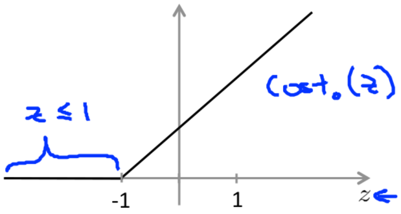


Figure 11: SVM cost_0

12.1.2 Support Vector Machine

Recall logistic regression has the form as in Equation 19, shown below in an alternate form (taking the negative sign into the summation):

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m}[y^{(i)} \;\; - log\, h_\theta(x^{(i)}) \;\; - (1-y^{(i)})\, log\,(\, 1 - h_\theta(x^{(i)})\,)\,] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

The Support Vector Machine has a similar form as logistic regression, with a few conventions that differ from its logistic regression counterpart:

1. Remove scaling term ($\frac{1}{m}$). Note that this does not change the final result of minimized θ.

2. The logistic regression has the form: $A + \lambda B$; the SVM has the form $CA + B$. This is just a different way of parametrizing tradeoffs. Note here C behaves similarly to $\frac{1}{\lambda}$.

Therefore, the SVM hypothesis can be expressed in Equation 31.

$$\underset{\theta}{min}\, C\sum_{i=1}^{m}[y^{(i)}\, cost_1(\theta^T x^{(i)}) + \;(1-y^{(i)})\, cost_0(\theta^T x^{(i)})] + \frac{1}{2}\sum_{j=1}^{n}\theta_j^2 \qquad (31)$$

The hypothesis

$$h_\theta(x) = \begin{cases} 1 & \text{if } \theta^T x \geq 0 \\ 0 & \text{if otherwise.} \end{cases}$$

12.2 Large Margin Intuition

Recall in Figure 10 and 11, we re-defined the function. Herein, we have shifted our threshold to z=1 and z=-1 respectively for predicting y = 1 and 0, respectively. This is different from previous threshold of 0 for logistic regression. We are more conservative in our predictions here, by using the 2 new segment cost functions, $\text{cost}_1(\theta^T x^{(i)})$ and $\text{cost}_0(\theta^T x^{(i)})$.

12.2.1 SVM Decision Boundary

Suppose we set C to be a large number, e.g. 10000. Under the minimization objective, we will be highly motivated to pick a θ such that the first term is close to zero, thus discarding the first term. The original equation will then be reduced effectively to

$$\underset{\theta}{min}\ \frac{1}{2}\sum_{j=1}^{n}\theta_j^2$$

such that

$$\theta^T x^{(i)} \begin{cases} \geq 1 & \text{if } y^{(i)} = 1 \\ \leq -1 & \text{if } y^{(i)} = 0 \end{cases}$$

12.2.2 Large Margin Classifier

The Support Vector Machine is also known as the Large Margin Classifier. The word margin refers to the distance between the boundary and the data points. SVM will try to maximize the distance, as seen in Figure 12.

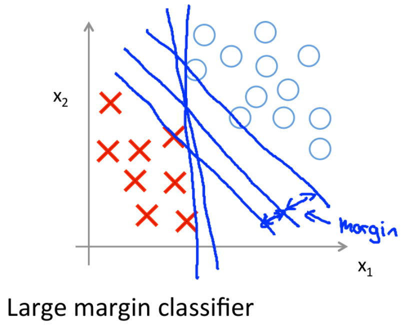


Figure 12: SVM Decision Boundary: Linearly Separable Case

When C is too large (similar to a small λ), then we get decrease the power of the margin margin classifier, and the algorithm will fit too well to outliers.

12.3 Kernels

12.3.1 Non-linear decision boundary

For a non-linear decision boundary problem (as shown in Figure 13), we have:

$$h_\theta = \begin{cases} 1, & \text{if } \theta_0 x + \theta_1 x_1 + \cdots \geq 0 \\ 0, & \text{otherwise} \end{cases}$$

This can be written as

$$\theta_0 x + \theta_1 f_1 + \theta_2 f_2 + \theta_3 f_3 + \ldots$$

, where

$$f_1 = x_1, f_2 = x_2, f_3 = x_1 x_2, f_4 = x_1^2, f_5 = x_2^2 \ldots$$

However, high order polynomials are expensive. Is there a better choice of features f_i's?

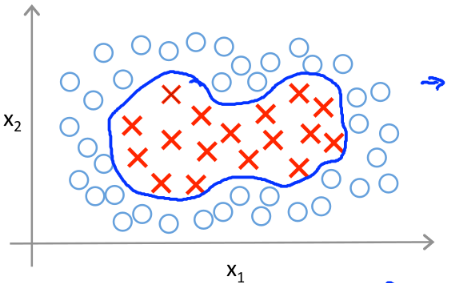


Figure 13: Nonlinear decision boundary problem

12.3.2 Kernel

Given x, compute new feature depending on proximity to landmarks $l^{(1)}, l^{(2)}, l^{(3)}$. This can be illustrated in Figure 14.

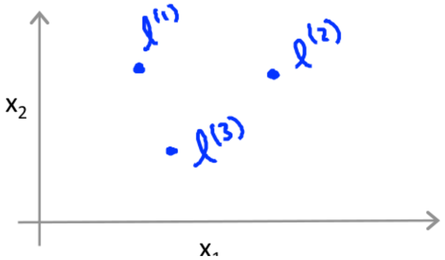


Figure 14: Kernel and landmark illustration

We then compute the features $f_i = kernel(x, l^{(i)})$ as follows:

$$f_i = \text{similarity}(x, l^{(i)}) = exp(-\frac{\|x - l^{(i)}\|^2}{2\sigma^2}) \tag{32}$$

This is a specific type of kernel, namely, the *Gaussian kernel*.

12.3.3 Kernels and Similarity

Note: The term $\|x - l^{(i)}\|$ in 32 can also be written as: $\sum_{j=1}^{n}(x^j - l_j^{(i)})^2$. We can analyze the term in two scenarios:

1. If $x \approx l^{(i)}$, then $\|x - l^{(i)}\| \approx 0$, consequently $f_i \approx 1$.
2. If x is far from $l^{(i)}$, then $\|x - l^{(i)}\|$ large, consequently $f_i \approx 0$.

Each landmark $l^{(i)}$ defines a new feature f_i, where the function approaches one when x is close to the landmark, and approaches zero otherwise.

The function can be visualized in Figure 15. Note that as the variance (σ) increases, f falls from the peak (1) slower.

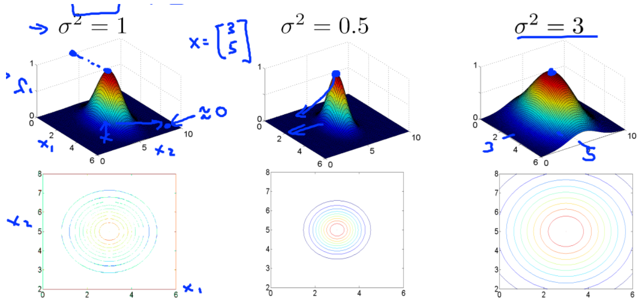


Figure 15: Guassian Kernel 3D plot

12.3.4 Choosing Landmark

A natural question arises: *Where do we get $l^{(i)}$?*

Recall from 32, given x we can compute a feature ($\mathrm{f_i}$) as the similarity between the point and the landmark.

We predict y = 1, when

$$\sum_{i}^{n} \theta_i f_i \geq 0$$

In practise, θ_0 is chosen to be negative, where $\theta_i, (i \neq 0)$ are chosen to be some non-negative constants. As such, the closer x_i is to each l_i, f_i will tend to 1, thus making the term $\theta_i f_i$ some positive number. We then take the sum of "weighted proximities to each landmark", and make the decision on y.

Observe Figure 16, where the markings of datasets we want is in blue, and red are the ones that we discard. Our goal is to guess what data belongs to our identification. Hence, we want to identify x that is close to our training examples.

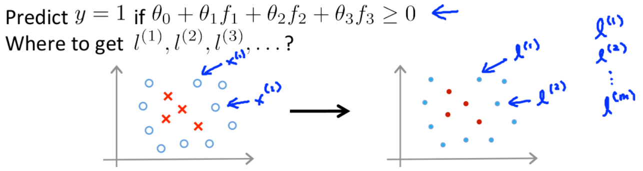

Predict $y = 1$ if $\theta_0 + \theta_1 f_1 + \theta_2 f_2 + \theta_3 f_3 \geq 0$
Where to get $l^{(1)}, l^{(2)}, l^{(3)}, \ldots$?
$x^{(1)}$
$x^{(2)}$
$l^{(1)}$
$l^{(2)}$
$l^{(1)}$
$l^{(2)}$
$l^{(m)}$

Figure 16: Landmark and Training dataset

Comparing the above two paragraphs, it follows naturally that we should choose the training examples as our landmarks. Thus features are a measure of *proximity to training examples*, given an x.

12.3.5 SVM with Kernels

A summary of our setup:

- Given training examples: $(x^{(i)}, y^{(i)})$, i $= 1 \ldots m$.
- Select landmarks: $l^{(i)} = x^{(i)}$
- Given example x: compute features $f_i = similarity(x, l^{(i)})$.
  For training example $(x^{(i)}, y^{(i)})$, where $x^{(i)} \in \mathbb{R}^{n+1}$ $(0 \ldots n)$. We can compute the feature vector $f^{(i)} \in \mathbb{R}^{m+1}$, where m is the number of landmarks (training examples).

$$f^{(i)} = \begin{bmatrix} f_0^{(i)} \\ f_1^{(i)} \\ f_2^{(i)} \\ \vdots \\ f_i^{(i)} \\ \vdots \\ f_m^{(i)} \end{bmatrix}$$

  1. $f_0^{(i)} = 1$ by default.
  2. $f_i^{(i)} = 1$ by design (check Equation 32; similarity of $x^{(i)}$ to $l^{(i)} = x^{(i)}$ is 1).

Formally:

1. **Hypothesis**: Given $x \in \mathbb{R}^{n+1}$, compute features $f \in \mathbb{R}^{m+1}$.
   Predict "y $= 1$", if $\theta^T f = \sum_{i=0}^{m} \theta_i f_i \geq 0$

2. **Training**:

$$\underset{\theta}{min}\, C \sum_{i=1}^{m} [y^{(i)}\, cost_1(\theta^T f^{(i)}) +\; (1-y^{(i)})\, cost_0(\theta^T f^{(i)})] + \frac{1}{2}\sum_{j=1}^{m} \theta_j^2$$

   Remarks:

   - The above equation is similar to 31.
   - We calculate the cost based on θ and f^i.
   - In the second summation, $n = m$; number of features=number of training sets.

3. **Implementation Note**

   - $\sum_{j=1}^{m} \theta_j^2 = \theta^T \theta; \theta = \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_m \end{bmatrix}$
   - Can also scale θ, i.e. $\theta^T M \theta$.
   - M increases computation efficiency.

12.3.6 SVM Parameters

We have two parameters: C and λ:

C$= \frac{1}{\lambda}$:

1. Large C (small λ): lower bias, higher variance.
2. Small C (large λ): Higher bias, low variance.

σ^2: (see Figure 15)

1. Large σ^2: (features f_i vary more smoothly) higher bias, lower variance.
2. Small σ^2: (changes abruptly) lower bias, higher variance.